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Advanced Molecular Quantum Mechanics: An Introduction to Relativistic Quantum Mechanics and the Quantum Theory of Radiation (Studies in Chemical Physics)

R. E. Moss

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This book is primarily intended for graduate chemists and chemical physicists. Indeed, it is based on a graduate course that I give in the Chemistry Depart ment of Southampton University. Nowadays undergraduate chemistry courses usually include an introduction to quantum mechanics with particular reference to molecular properties and there are a number of excellent textbooks aimed specifically at undergraduate chemists. In valence theory and molecular spectroscopy physical concepts are often encountered that are normally taken on trust. For example, electron spin and the anomalous magnetic moment of the electron are usually accepted as postulates, although they are well understood by physicists. In addition, the advent of new techniques has led to experimental situations that can only be accounted for adequately by relatively sophisticated physical theory. Relativis tic corrections to molecular orbital energies are needed to explain X-ray photo electron spectra, while the use oflasers can give rise to multiphoton transitions, which are not easy to understand using the classical theory of radiation. Of course, the relevant equations may be extracted from the literature, but, if the underlying physics is not understood, this is a practice that is at best dissatisfy ing and at worst dangerous. One instance where great care must be taken is in the use of spectroscopically determined parameters to test the accuracy of elec tronic wave functions.

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